

A Dispersion Relation for the Density of States With Application to the Casimir Effect

S. G. Rajeev

Department of Physics and Astronomy

Department of Mathematics

University of Rochester

Rochester, NY 14627, USA

Abstract

The trace of a function of a Schrödinger operator minus the same for the Laplacian can be expressed in terms of the determinant of its scattering matrix. The naive formula for this determinant is divergent. Using a dispersion relation, we find another expression for it which is convergent, but needs one piece of information beyond the scattering matrix. Except for this ‘anomaly’, we can express the Casimir energy of a compact body in terms of its optical scattering matrix, without assuming any rotational symmetry for its shape.

1 Introduction

The kinetic theory of gases in classical physics predicts that every surface in a gas is bombarded by molecules. The recoil of these molecules exert a pressure on the surface. A spectacular demonstration of this prediction would be to evacuate the air inside an aluminium can: there will be a net inward pressure that will cause the can to collapse.

In the quantum theory of fields, there is an analogous pressure on every surface that can scatter light[1, 2]. Even in the vacuum there are ‘virtual photons’ which describe the quantum fluctuations of the electromagnetic field in its ground state. These virtual photons are scattered by any medium that can interact with light; this scattering exerts a force on the medium. Although quite small in magnitude, it has been measured experimentally[3].

In the original calculation of the Casimir force only simple shapes such as a sphere, or a rectangular slab were studied. Moreover, the medium was assumed to have ideal properties, such as perfect conductivity. Since that time, new methods have been developed, which allow the calculation of the Casimir energy for more general shapes. Of particular interest to us are the spectral methods[4, 5, 6, 7, 8] . (Methods that allow realistic computation of Casimir energy of micro-electromechanical or MEM devices have been developed recently[9]; but we do not use them in this paper.) The basic idea behind these methods is a relationship (often called Levinson’s theorem or Krein’s trace formula) between the optical scattering matrix S and the density of states:

$$\rho(k) = \frac{1}{2\pi i} \frac{d}{dk} \text{tr} \log S, \quad (1)$$

The Casimir energy is the sum over frequencies weighted by $\rho(k)$.

The physical argument that the Casimir force is due to the reflection of virtual photons suggests that it should be possible to express it entirely in terms of the probability of reflection. Unless the momentum of the photon changes during scattering, it should not contribute to the Casimir force.

In this paper we will show that the dispersion relations of scattering theory allow an answer for the density of states in terms of the reflection probability alone, in the one dimensional case. In the three dimensional case, there is a potential logarithmic divergence in $\text{tr} \log S$. We show how to remove this by using a dispersion relation, without assuming rotational symmetry or using perturbation theory as in previous treatments [10]. An outcome is an ‘anomaly’ term in the density of states proportional to the integral of the potential. Contrary to the physical picture in terms of scattering of virtual photons, there is this one contribution to the Casimir effect that cannot be expressed in terms of the scattering matrix alone.

Much of our detailed analysis will be only carried out for the technically simpler case of a scalar field. As in traditional optical scattering theory, this scalar model gives a reasonable picture of the essential phenomenon. It is straightforward although technically involved to extend our analysis to include polarization effects; i.e., scattering of vectorial fields. Moreover, we will ignore the effects of absorption of light: the effect of absorption on virtual photons needs a deeper analysis than we can provide at the moment. Also, we will consider only optical media that are time independent. For a technical reason, we will further assume that the scatterer is parity invariant; although it does not have to be symmetric otherwise.

We aim to give a more or less self-contained description, taking off from the discussion of scattering in standard textbooks. The erudite reader could skip ahead to sections 3.1,3.2 and 5. No pretense at mathematical rigor is made. However, there will be an occasion for us to be careful about the definition of an infinite determinant (of the scattering operator) to avoid a logarithmic divergence.

2 Scattering of Light

The propagation of light of(Ref. [11]) wave-number k in a dielectric medium is described by the equations

$$\nabla \times \mathbf{E} = ik\mathbf{H}, \quad \nabla \times \mathbf{H} = -ik\epsilon(x, k)\mathbf{E}. \quad (2)$$

Here, $\epsilon(x, k)$ is the dielectric ‘constant’ which may in fact depend on position and on the wave-number k . (In other words, $\epsilon(x, k)$ is the square of the refractive index.) \mathbf{E} and \mathbf{H} are complex vector valued functions describing the amplitude of the electromagnetic wave.

Eliminating \mathbf{H} , we get

$$\nabla \times \nabla \times \mathbf{E}(x, k) = k^2\epsilon(x, k)\mathbf{E}. \quad (3)$$

In other words,

$$\nabla \times \nabla \times \mathbf{E}(x, k) + V(x)\mathbf{E} = k^2\mathbf{E} \quad (4)$$

where the ‘effective potential’ [12] is

$$V(x) = k^2[1 - \epsilon(x, k)]. \quad (5)$$

There is an analogy between the above equation describing the classical scattering of light and the quantum mechanical scattering of a particle by a potential. The Schrödinger equation (in natural units $\hbar = 2m = 1$) is

$$-\nabla^2\psi + V(x)\psi = k^2\psi. \quad (6)$$

The essential difference is that the vector Laplacian $\nabla \times \nabla \times \mathbf{E}$ is replaced by the scalar Laplacian ∇^2 . The potential $V(x)$ is related to the refractive index as in the formula above. If the refractive index is less than one, the ‘potential’ is positive; this is the case for large enough k .

Thus it will be useful to use the language of quantum mechanical scattering theory, although of course the scattering we are talking about is just the classical scattering of light waves. But some differences must be kept in mind. For example, the ‘potential’ $V(x, k)$ will depend on wavenumber, a fact that has no simple meaning in quantum mechanics. The wave-number dependence of the scattering matrix will be affected by this dispersion of the light waves. Our final formulas only involve the scattering matrix and thus take into account of this effect. But we will often not explicitly display the dependence of the potential on the wavenumber.

3 Waves in 1 + 1 Dimensions

We will start our discussion in the simplest possible case, the scalar theory in one space and one time. We will later generalize the ideas to three dimensions and to vector waves, but it is pedagogically useful to start with the simplest case.

Often we are interested in deriving a formula for the sum over a function ϕ of the eigenvalues of a hamiltonian operator H . This can be thought of as the trace of an operator $\text{tr } \phi(\sqrt{H})$. For example, the Casimir energy of a massless scalar field in the presence of an external potential is $\text{tr } \sqrt{H}$. Another example is the thermodynamic partition function, $\text{tr } e^{-\beta H}$. More precisely we will be interested in the difference between this trace and its value for the free hamiltonian.

With this in mind, let

$$H = -\frac{d^2}{dx^2} + V(x), \quad H_0 = -\frac{d^2}{dx^2} \quad (7)$$

We can think of H be as the Schrödinger operator of a one dimensional quantum mechanical system. The potential $V(x)$ is positive, smooth and vanishes faster than any power of x at infinity. Thus, $H \geq 0$.

Let $\phi(k)$ be a smooth function on $[0, \infty)$ which vanishes at infinity faster than k^{-1} . We are going to derive a formula for the quantity

$$\bar{\text{tr}} \phi(\sqrt{H}) = \text{tr} [\phi(\sqrt{H}) - \phi(\sqrt{H_0})]. \quad (8)$$

We assume, for now, that $\phi(k)$ vanishes for large k : postponing the study of ultraviolet divergences. We might expect that there is an integral representation

$$\bar{\text{tr}} \phi(\sqrt{H}) = \int_0^\infty \phi(k) \rho(k) dk. \quad (9)$$

We will get a formula for the ‘spectral density’ $\rho(k)$ in terms of the scattering matrix. We can get this directly from the formula for the resolvent in terms of the Jost functions[5, 6], but we will give a more physical but less rigorous argument.

Instead, we will look at the continuous spectrum as the limit of an eigenvalue problem. Imagine we have enclosed the whole system in a box of size $2L$: we require that the eigenfunctions of H and H_0 vanish at $x = \pm L$. Then we have a discrete number of allowed values of momentum, $k_n(L)$. For example when $V(x) = 0$, they are $\frac{\pi n}{2L}$. Thus

$$\bar{\text{tr}} \phi(\sqrt{H}) = \sum_n \left[\phi(k_n(L)) - \phi\left(\frac{\pi n}{2L}\right) \right] \quad (10)$$

This sum will become an integral in the limit as $L \rightarrow \infty$. Even when L is kept finite, we can assume that it is much larger than the range of the potential $V(x)$, since we are only interested in the limit $L \rightarrow \infty$.

At infinity, the solutions of the Schrödinger equation [13]

$$-u'' + V(x)u(x) = k^2 u(x) \quad (11)$$

tend to a sum of plane waves:

$$\begin{aligned} u(x) &\rightarrow Ae^{ikx} + Be^{-ikx} \text{ for } x \rightarrow -\infty \\ &\rightarrow Ce^{ikx} + De^{-ikx} \text{ for } x \rightarrow \infty. \end{aligned} \quad (12)$$

Thus A, D are the amplitudes of the incoming waves and C, B those of the outgoing waves. Conservation of probability gives

$$|A|^2 + |D|^2 = |C|^2 + |B|^2. \quad (13)$$

Since the Schrödinger equation is a second order differential equation, there are two constants of integration in its general solution. Let us choose them to be A and D , the amplitudes of the incoming waves. Then the amplitudes

of the outgoing waves are determined once we solve the differential equation:

$$\begin{pmatrix} C \\ B \end{pmatrix} = S(k) \begin{pmatrix} A \\ D \end{pmatrix}. \quad (14)$$

The matrix $S(k)$ is unitary from the conservation of probability: it is the scattering matrix associated to the potential V .

Often we describe the scattering in terms of reflection and transmission coefficients. They are defined by the special choice $A = 1, D = 0$ corresponding to waves incident from the left:

$$\begin{aligned} u(x) &\rightarrow e^{ikx} + R(k)e^{-ikx} \text{ for } x \rightarrow -\infty \\ &\rightarrow T(k)e^{ikx} \text{ for } x \rightarrow \infty. \end{aligned} \quad (15)$$

Taking complex conjugate we have another solution,

$$\begin{aligned} u^*(x) &\rightarrow e^{-ikx} + R^*(k)e^{ikx} \text{ for } x \rightarrow -\infty \\ &\rightarrow T^*(k)e^{-ikx} \text{ for } x \rightarrow \infty. \end{aligned} \quad (16)$$

Taking linear combinations, gives the solution describing waves incident from the right:

$$\begin{aligned} \frac{u^*(x) - R^*(k)u(x)}{T^*(k)} &\rightarrow \frac{1 - |R(k)|^2}{T^*(k)} e^{-ikx} \text{ for } x \rightarrow -\infty \\ &\rightarrow -\frac{R^*(k)T(k)}{T^*(k)} e^{ikx} + e^{-ikx} \text{ for } x \rightarrow \infty. \end{aligned} \quad (17)$$

Thus (recalling that $|R(k)|^2 + |T(k)|^2 = 1$),

$$S(k) = \begin{pmatrix} T(k) & -R^*(k)\frac{T(k)}{T^*(k)} \\ R(k) & T(k) \end{pmatrix} \quad (18)$$

We might check explicitly that this matrix is unitary.

Being unitary, there is a basis in which $S(k)$ is diagonal, with eigenvalues $e^{2i\eta_{1,2}(k)}$. The real valued functions $\eta_{1,2}(k)$ are the ‘phase shifts’ of the scattering problems.

Now let us return to the eigenvalue problem

$$-u'' + V(x)u(x) = k^2u(x), \quad u(-L) = u(L) = 0 \quad (19)$$

Since L is large compared to the range of $V(x)$, we can use the asymptotic forms above in the boundary conditions:

$$Ae^{-ikL} + Be^{ikL} = 0 = Ce^{ikL} + De^{-ikL}. \quad (20)$$

Solving for B and C ,

$$B = -Ae^{-2ikL}, \quad C = -De^{-2ikL}. \quad (21)$$

Thus the momenta k are determined by the equation

$$S(k) \begin{pmatrix} A \\ D \end{pmatrix} = -e^{-2ikL} \begin{pmatrix} D \\ A \end{pmatrix}. \quad (22)$$

So far we are in arbitrary basis in the two dimensional space of solutions.

Now let us choose this basis to the one that diagonalizes $S(k)$:

$$e^{2i\eta_1(k)}A = -e^{-2ikL}D, \quad e^{2i\eta_2(k)}D = -e^{-2ikL}A. \quad (23)$$

Eliminating D ,

$$e^{2i[\eta_1(k)+\eta_2(k)+2kL]} = 1. \quad (24)$$

This is the transcendental equation for the allowed wavenumbers,

$$k = \frac{\pi n}{2L} - \frac{\eta_1(k) + \eta_2(k)}{2L}, \text{ for } n = \dots - 2, -1, 0, 1, 2, \dots \quad (25)$$

Since L is very large in the limit we are interested in, the second term is a small correction. It is enough to solve the equation approximately by iterating it once:

$$k_n(L) = \frac{\pi n}{2L} - \frac{\eta_1(\frac{\pi n}{2L}) + \eta_2(\frac{\pi n}{2L})}{2L} \quad (26)$$

We can now reexpress the sum over phase shifts in terms of the Scattering matrix:

$$2i[\eta_1(k) + \eta_2(k)] = \log \det S(k). \quad (27)$$

For later use we also note that,

$$\det S(k) = T^2(k) + \frac{|R(k)|^2 T(k)}{T^*(K)} = \frac{T(k)}{T^*(k)} \quad (28)$$

so that

$$\log \det S(k) = 2i \arg T(k). \quad (29)$$

Thus,

$$k_n(L) - \frac{\pi n}{2L} = -\frac{\log \det S(\frac{\pi n}{2L})}{4iL} \quad (30)$$

Now we are ready to evaluate the sum over momenta in the limit as $L \rightarrow \infty$.

$$\begin{aligned} \bar{\text{tr}} \phi(\sqrt{H}) &= \sum_n \left[\phi(k_n(L)) - \phi\left(\frac{\pi n}{2L}\right) \right] \\ &= -\sum_n \phi'\left(\frac{\pi n}{2L}\right) \frac{\log \det S(\frac{\pi n}{2L})}{4iL} \end{aligned} \quad (31)$$

This becomes an integral as $L \rightarrow \infty$:

$$\bar{\text{tr}} \phi(\sqrt{H}) = -\int_0^\infty \frac{dk}{2\pi i} \frac{d\phi(k)}{dk} \log \det S(k) \quad (32)$$

Similar trace formulas have been derived by many other methods[5, 6, 10].

If the potential is independent of frequency, the integral will converge if $\phi(k)$ falls off faster than k^{-1} for large k and remains finite for small k . (This is because $T(k) \sim 1 + \frac{1}{2ik} \int V(x)dx$ for large k from the Born approximation; more on this later.) If $\phi(k)$ does not fall off at large k , the integral can still converge if $V(x, k)$ tends to zero for large $|k|$, so that $S(k)$ tends to unity faster also.

Even if the potential depends on the wave-number, it will still determine a unitary scattering matrix $S(k)$ for each k . We can still ask for the sum over the allowed values of wave-number for finite L as before; it is determined by the same formula in terms of the scattering matrix. Indeed, the whole argument goes through without any change.

3.1 Dispersion Relation

We will now express the density of states in terms of the reflection coefficient. The force due to the scattering of a virtual particle ought to be dependent on the probability of reflection: if the particle is transmitted, its momentum does not change and hence it should exert no force. Thus it is physically unsatisfactory that we have a formula in terms of the argument of the transmission amplitude rather than the magnitude of the reflection amplitude.

But we now remember the basic fact that $T(k)$ is analytic in the upper half plane. There are no poles since there are no bound states. Moreover, $T(k)$ never has zeros in the upper half plane. Hence $\log T(k)$ is also analytic in the upper half plane. There is then a dispersion relation [13] between its

real and imaginary parts (Hilbert transform) :

$$\text{Im } \log T(k) = \frac{1}{\pi} \mathcal{P} \int \frac{\text{Re } \log T(k')}{k' - k} dk'. \quad (33)$$

But

$$\text{Re } \log T(k) = \frac{1}{2} \log |T(k)|^2 = \frac{1}{2} \log[1 - |R(k)|^2]. \quad (34)$$

Thus

$$\arg \det S(k) = 2 \arg T(k) = \mathcal{P} \int \frac{\log[1 - |R(k')|^2]}{k' - k} \frac{dk'}{\pi}. \quad (35)$$

3.2 The Trace In Terms of the Reflection Coefficient

Combining the above results we get

$$\bar{\text{tr}} \phi(\sqrt{H}) = - \int_0^\infty \frac{dk}{2\pi} \frac{d\phi(k)}{dk} \arg \det S(k) \quad (36)$$

$$= \mathcal{P} \int_0^\infty \frac{dk}{2\pi} \int_{-\infty}^\infty \frac{dk'}{\pi} \frac{d\phi(k)}{dk} \frac{\log[1 - |R(k')|^2]}{k - k'} \quad (37)$$

Assuming parity invariance $|R(k)| = |R(-k)|$,

$$\bar{\text{tr}} \phi(\sqrt{H}) = \mathcal{P} \int_0^\infty \frac{dk}{\pi} \frac{dk'}{\pi} \frac{d\phi(k)}{dk} \frac{k \log[1 - |R(k')|^2]}{k^2 - k'^2} \quad (38)$$

We can expand the log in a power series to get a ‘multiple reflection expansion’ for this quantity.

When $\phi(k) = k$ this can be simplified to

$$\bar{\text{tr}} \sqrt{H} = \frac{1}{2} \int_0^\infty \frac{dk}{\pi} \frac{dk'}{\pi} \frac{k \log[1 - |R(k')|^2] - k' \log[1 - |R(k)|^2]}{k^2 - k'^2} \quad (39)$$

with a non-singular integrand.

4 Waves in 3 + 1 Dimensions

Consider the operator $H = -\nabla^2 + V(x)$, on $L^2(R^3)$ where the ‘potential’ $V(x)$ is a real function on R^3 that vanishes at infinity. (The potential also can depend on the wave-number: but again we don’t display this explicitly.) We will also assume for simplicity that that H has positive continuous spectrum ; i.e., that it has no ‘bound states’.

We will again be interested in the the difference

$$\bar{\text{tr}}(\phi(\sqrt{H})) = \text{tr } \phi(\sqrt{H}) - \text{tr } \phi(\sqrt{H_0}) \quad (40)$$

of the trace from that with the free hamiltonian:

$$H_0 = -\nabla^2. \quad (41)$$

The function $\phi(k)$ will, to begin with, be assumed to be smooth and vanish at infinity faster than k^{-3} : this is necessary to avoid ‘ultra-violet’ divergences. Later on we will allow for $\phi(k) = k$ and check that the integrals converge when the wave number dependence of the potential is take into account. Again we will derive a formula that involves the scattering matrix.

Since the potential vanishes at infinity, there is a solution to the equation

$$[-\nabla^2 + V(x)]\psi(x) = k^2\psi(x) \quad (42)$$

that tend to a sum of a plane wave and an outgoing spherical wave[13]:

$$\psi(r, \mathbf{n}') \rightarrow e^{ikr\mathbf{n}\cdot\mathbf{n}'} + f(k, \mathbf{n}, \mathbf{n}')\frac{e^{ikr}}{r}, \quad \text{as } r \rightarrow \infty \quad (43)$$

Here, \mathbf{n} is the direction of the incoming plane wave and \mathbf{n}' the direction along which we let the argument of the wavefunction go to infinity. The function $f(k, \mathbf{n}, \mathbf{n}')$ is the scattering amplitude.

Since there are no bound states, the general solution can be written as a superposition of such scattering solutions, [13] weighted by a function $F(\mathbf{n})$ of the direction of incidence. Such a general solution will have the asymptotic behavior at spatial infinity,

$$\psi_F(r, \mathbf{n}') \sim \int F(\mathbf{n}) e^{ikr\mathbf{n}\cdot\mathbf{n}'} d\Omega_{\mathbf{n}} + \frac{e^{ikr}}{r} \int F(\mathbf{n}) f(k, \mathbf{n}, \mathbf{n}') d\Omega_{\mathbf{n}} \quad (44)$$

As $r \rightarrow \infty$ the first integral can be evaluated by the method of steepest descents, to get

$$2\pi i F(-\mathbf{n}') \frac{e^{-ikr}}{kr} - 2\pi i F(\mathbf{n}') \frac{e^{ikr}}{kr}. \quad (45)$$

Thus we can write

$$\psi_F(r, \mathbf{n}') \sim \frac{2\pi i}{k} \left\{ \frac{e^{-ikr}}{r} F(-\mathbf{n}') - \frac{e^{ikr}}{r} [1 + 2ik\hat{f}(k)F](\mathbf{n}') \right\} \quad (46)$$

where $\hat{f}(k)$ is the operator on $L^2(S^2)$:

$$\hat{f}(k)F(\mathbf{n}') = \frac{1}{4\pi} \int f(k, \mathbf{n}, \mathbf{n}') F(\mathbf{n}) d\Omega_{\mathbf{n}}. \quad (47)$$

The quantity

$$\hat{S}(k) = 1 + 2ik\hat{f}(k) \quad (48)$$

is the scattering operator. Conservation of probability requires it to be unitary.

Being unitary this operator can be diagonalized on $L^2(S^2)$. If H is spherically symmetric, the eigenfunctions of \hat{S} are the spherical harmonics:

$$\hat{S}(k)Y_{lm}(\mathbf{n}) = e^{2i\eta_l(k)}Y_{lm}(\mathbf{n}). \quad (49)$$

The eigenvalues are determined by the ‘phase-shifts’ $\eta_l(k)$ in each angular momentum sector. Even if H is not spherically symmetric, there will be

some spectrum of ‘phase shifts’ $\eta_a(k)$:

$$\hat{S}(k)\chi_a(k, \mathbf{n}) = e^{2i\eta_a(k)}\chi_a(k, \mathbf{n}). \quad (50)$$

(We will assume for now that this spectrum of \hat{S} is discrete; i.e., that the label a takes values in a countable set.)

Let us first imagine that our whole system is enclosed in a spherical box of large radius R with the wavefunction required to vanish on this surface. (The exact shape doesn’t matter in the limit $R \rightarrow \infty$, which is all we are interested in, so we might as well assume it is spherical.) For finite R there is a discrete set of allowed values for k , say $k_{na}(R)$. They are fixed by the condition

$$\psi(R, \mathbf{n}') = 0. \quad (51)$$

When R is large, this becomes,

$$\hat{S}(k)F(\mathbf{n}) = e^{-2ikR}F(-\mathbf{n}). \quad (52)$$

By squaring,

$$\hat{S}(k)^2 F(\mathbf{n}) = e^{-4ikR} F(\mathbf{n}) \quad (53)$$

Not every solution of (53) is a solution of (52). In the limit of large R , we can take account of this over-counting just dividing the density of states by two¹.

¹For example, in the spherically symmetric case each solution is degenerate, with degeneracy labelled by the angular momentum quantum numbers. In order to satisfy (52), we have the additional condition that n is odd for odd angular momentum l and even for even l . This is not needed for (53)

The solutions of (53) are the eigenfunctions of the scattering matrix introduced above; the momenta are fixed by

$$4\eta_a(k) + 4kR = 2\pi n, \quad n = 0, 1, 2, \dots \quad (54)$$

Thus, the solutions are labelled by n, a and will depend on R : $k_{na}(R)$. In the case of the free particle, the phase shifts vanish and the allowed momentum values are

$$\frac{\pi n}{2R}. \quad (55)$$

As R becomes large the solutions will differ from this by a small correction:

$$k_{na}(R) = \frac{\pi n}{2R} + \frac{q_{na}(R)}{R}. \quad (56)$$

We get

$$q_{na}(R) = -\eta_a\left(\frac{\pi n}{2R}\right). \quad (57)$$

Now consider the difference of traces, (remembering to divide by two to avoid the above mentioned over-counting)

$$\bar{\text{tr}} \phi(\sqrt{H}) = \frac{1}{2} \sum_{n,a} \left[\phi(k_{na}(R)) - \phi\left(\left\{\frac{\pi n}{2R}\right\}\right) \right]. \quad (58)$$

As $R \rightarrow \infty$ we get

$$\bar{\text{tr}} \phi(\sqrt{H}) = -\frac{1}{2R} \sum_{n,a} \phi'(k) \eta_a\left(\frac{\pi n}{2R}\right) \rightarrow -\sum_a \int_0^\infty \frac{dk}{\pi} \frac{d\phi(k)}{dk} \eta_a(k). \quad (59)$$

In other words,

$$\bar{\text{tr}} \phi(\sqrt{H}) = -\frac{1}{2\pi i} \int dk \frac{d\phi(k)}{dk} \text{tr} \log \hat{S}(k). \quad (60)$$

We are thinking of $\hat{S}(k)$ as an operator on $L^2(S^2)$, so the trace on the r.h.s. is the average over angles. We will now turn to a more precise definition of this trace: naively it is logarithmically divergent.

4.1 A toy model: the Gamma function

The reader familiar with the theory of modified determinants as in equation (67) below could skip this subsection.

Recall that the Gamma function has poles at negative integers and zero; its reciprocal is an entire function with zeroes at these points. So we might hope for a product formula

$$\frac{1}{\Gamma(z)} \sim z \prod_{n=1}^{\infty} \left[1 + \frac{z}{n} \right] \quad (61)$$

Alas, this product is divergent: the product $\prod_n [1 + \lambda_n]$ converges when the sum $\sum_n |\lambda_n|$ converges. In the our case, $\sum_n \frac{1}{n}$ diverges logarithmically. But, the sum of the squares converges: $\sum_n \frac{1}{n^2} < \infty$.

This suggests a fix to this divergence problem. The function $e^{-z}(1+z)$ has the same zero as $1+z$ but tends to one faster as $|z| \rightarrow 0$.

Indeed, $|e^{-z}(1+z) - 1| < C|z|^2$. So the product

$$\prod_{n=1}^{\infty} e^{-\frac{z}{n}} \left[1 + \frac{z}{n} \right] \quad (62)$$

converges. So we can separate out a divergent part of (66) as follows:

$$\log \frac{1}{\Gamma(z)} = \log z + \sum_{n=1}^{\infty} \log \left\{ e^{-\frac{z}{n}} \left[1 + \frac{z}{n} \right] \right\} + z \sum_{n=1}^{\infty} \frac{1}{n} \quad (63)$$

The divergence has been isolated to the last term. How to give a meaning to that last divergent sum? We might guess that the correct formula is

$$\log \frac{1}{\Gamma(z)} = \log z + \sum_{n=1}^{\infty} \log \left\{ e^{-\frac{z}{n}} \left[1 + \frac{z}{n} \right] \right\} + az \quad (64)$$

for some constant a ; and determine it by comparison with the value of the logarithmic derivative of $\Gamma(z)$ at some point. This is a kind of renormalization

of the logarithmic divergence. Indeed, we know that

$$\psi(z) \equiv \frac{d}{dz} \log \Gamma(z) \sim -\frac{1}{z} - \gamma + O(z) \quad (65)$$

where γ is the Euler constant. Thus we conclude that $a = \gamma$:

$$\frac{1}{\Gamma(z)} = ze^{\gamma z} \prod_{n=1}^{\infty} e^{-\frac{z}{n}} \left[1 + \frac{z}{n} \right] \quad (66)$$

This argument would not pass muster with a modern analyst. But it is precisely such heuristic arguments that led to the rigorous modern theory of analytic functions. Quantum Field Theory is still in the stage of development that complex function theory was in the mid nineteenth century: we need to work with heuristic, physically motivated arguments which point the way to the truth. These then should be turned into theorems later, as stronger constructive methods become available.

4.2 Infinite Determinants

The determinant of an operator $1 + X$ is well-defined when X is trace-class: that is, when the sum of the absolute values of its characteristic values is convergent. But the scattering matrices of interest to us are not this type: $\hat{S} - 1$ is not trace-class. However, we will see soon that it has the next best property: the sum of the absolute squares of the characteristic values of $\hat{S} - 1$ converges, because it is proportional to the total scattering cross-section. When X is Hilbert-Schmidt (i.e., $\text{tr } X^\dagger X < \infty$), the modified determinant [14, 15]

$$\det_1 [1 + X] = \det e^{-X} [1 + X] \quad (67)$$

is meaningful. (The point is that the analytic function $e^{-z}(1+z) - 1$ is bounded by $c|z|^2$ for some constant c . Hence $e^{-X}[1+X] - 1$ is trace-class if X is Hilbert-Schmidt.) Now, we can write the logarithm of the original determinant as

$$\log \det[1+X] = \log \det_1[1+X] + \operatorname{tr} X \quad (68)$$

which separates out the divergent term $\operatorname{tr} X$.

Lemma $\hat{S}(k) - 1$ is Hilbert-Schmidt

Proof: In terms of the scattering amplitude,

$$\operatorname{tr} (\hat{S}(k) - 1)^\dagger (\hat{S}(k) - 1) = 4k^2 \operatorname{tr} \hat{f}^\dagger \hat{f} = 4k^2 \int |f(k, \mathbf{n}, \mathbf{n}')|^2 \frac{d\Omega_{\mathbf{n}} d\Omega_{\mathbf{n}'}}{(4\pi)^2} \quad (69)$$

But the total cross-section for a beam incident along the direction \mathbf{n} is

$$\sigma(k, \mathbf{n}) = \int |f(k, \mathbf{n}, \mathbf{n}')|^2 d\Omega_{\mathbf{n}'}. \quad (70)$$

Thus

$$\operatorname{tr} (\hat{S}(k) - 1)^\dagger (\hat{S}(k) - 1) = \frac{1}{\pi} k^2 \bar{\sigma}(k) \quad (71)$$

where

$$\bar{\sigma}(k) = \frac{1}{4\pi} \int d\Omega_{\mathbf{n}} \sigma(k, \mathbf{n}) \quad (72)$$

is the average total cross-section, which is finite as was promised.

Then $(1 + 2ik\hat{f})e^{-2ik\hat{f}} - 1$ is a trace-class operator and the modified determinant $\det_1 \hat{S}(k)$ defined by [14]

$$\det_1[\hat{S}(k)] = \det[(1 + 2ik\hat{f})e^{-2ik\hat{f}}] \quad (73)$$

exists. Moreover we have the bound,

$$|\log \det_1[\hat{S}(k)]| < \frac{1}{2} \operatorname{tr} [\hat{S}(k) - 1]^\dagger [\hat{S}(k) - 1] = \frac{1}{2\pi} k^2 \bar{\sigma}(k) \quad (74)$$

which will be useful later.

We can write

$$\log \det \hat{S}(k) = \log \det_1 \hat{S}(k) + 2ik \operatorname{tr} \hat{f}(k). \quad (75)$$

The real parts of the terms on the l.h.s must cancel, since the scattering matrix is unitary. So we might as well write,

$$\log \det \hat{S}(k) = i \operatorname{Im} \log \det_1 \hat{S}(k) + 2ik \operatorname{Re} \operatorname{tr} \hat{f}(k). \quad (76)$$

5 A Dispersion Relation

The last term, which is potentially divergent, can be given a meaning using the dispersion relation which relates it to the scattering cross-section:(See [13])

$$\operatorname{Re} \operatorname{tr} \hat{f}(k) = -\frac{1}{2\pi} \int V(x, k) d^3x + \frac{1}{4\pi^2} \mathcal{P} \int_0^\infty \frac{2k'^2 \bar{\sigma}(k')}{k'^2 - k^2} dk'. \quad (77)$$

(Here, \mathcal{P} stands for the principal part of the integral.) The first term is just the Born approximation of the forward scattering amplitude. We will see in a minute that

$$\bar{\sigma}(k) \sim k^{-2}, \text{ as } k \rightarrow \infty. \quad (78)$$

(This is for the case that the potential $V(x)$ is independent of k . It falls off even faster if the potential itself vanishes for large k .) Hence this integral is

convergent. Thus we have the formula we seek:

$$\arg \det \hat{S}(k) = \arg \det_1 \hat{S}(k) - \frac{k}{\pi} \int V(x, k) d^3x + \frac{k}{\pi^2} \mathcal{P} \int_0^\infty \frac{k'^2 \bar{\sigma}(k')}{k'^2 - k^2} dk'. \quad (79)$$

As in (37) we can now get trace of a function of the hamiltonian:

$$\bar{\text{tr}} \phi(\sqrt{H}) = \int_0^\infty \frac{dk}{2\pi} \frac{d\phi(k)}{dk} \frac{k}{\pi} \int V(x, k) d^3x \quad (80)$$

$$- \int_0^\infty \frac{dk}{2\pi} \frac{d\phi(k)}{dk} \frac{k}{\pi^2} \mathcal{P} \int_0^\infty \frac{k'^2 \bar{\sigma}(k')}{k'^2 - k^2} dk' \quad (81)$$

$$- \int_0^\infty \frac{dk}{2\pi} \frac{d\phi(k)}{dk} \arg \det_1 S(k) \quad (82)$$

$$(83)$$

The last term, which is the most complicated to calculate, can be bounded (74) by the total cross-section :

$$\left| \int_0^\infty \frac{dk}{2\pi} \frac{d\phi(k)}{dk} \arg \det_1 S(k) \right| < \int_0^\infty \frac{dk}{2\pi} \frac{d\phi(k)}{dk} \frac{k^2 \bar{\sigma}(k)}{2\pi} \quad (84)$$

5.1 Application to Casimir Energy

An application of the above formula is to the Casimir effect, $\phi(k) = k$. To avoid divergences, we assume that

$$k^2 V(x, k) \rightarrow 0 \quad (85)$$

for large k .

$$\bar{\text{tr}} \sqrt{H} = \int_0^\infty \frac{dk}{2\pi} \frac{k}{\pi} \int V(x, k) d^3x \quad (86)$$

$$- \int_0^\infty \frac{dk}{2\pi} \frac{dk'}{2\pi} \frac{kk'}{\pi} \frac{k' \bar{\sigma}(k') - k \bar{\sigma}(k)}{k'^2 - k^2} \quad (87)$$

$$- \int_0^\infty \frac{dk}{2\pi} \arg \det_1 \hat{S}(k) \quad (88)$$

The first two terms should give a good approximation in many cases. Again, the last term can be bounded by the cross-section,

$$\left| \int_0^\infty \frac{dk}{2\pi} \arg \det_1 S(k) \right| < \int_0^\infty \frac{dk}{2\pi} \frac{k^2 \bar{\sigma}(k)}{2\pi} \quad (89)$$

The computation of the scattering matrix from the optical potential is a separate problem: it can be done numerically. Or we could measure the scattering matrix experimentally and use it directly to calculate the Casimir energy.

Despite the physical intuition that the Casimir force is due to reflection of virtual photons, we do not get an answer entirely in terms of the scattering matrix: the first term involves the potential itself. This is similar to the way that the product formula for the Gamma function does not just involve the location of its poles: our term involving the potential is the analogue of the term involving the Euler constant in the formula for $\log \Gamma(z)$. Such ‘anomalies’ occur elsewhere in Quantum Field Theory[16] as well.

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